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(*E*)-2-Phenylbenzaldehyde oxime forms hydrogen-bonded $C_2^2(6)$ chains

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.007 Å
R factor = 0.045
wR factor = 0.111
Data-to-parameter ratio = 8.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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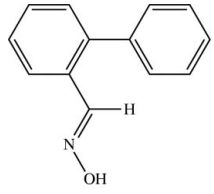
The title compound, $C_{13}H_{11}NO$, crystallizes in space group $Pca2_1$ with $Z' = 2$. The molecules are linked by two N—H···O hydrogen bonds [H···O = 1.96 and 1.97 Å, N···O = 2.789 (4) and 2.799 (4) Å, and N—H···O both 171°] into $C_2^2(6)$ chains.

Comment

The title compound, (I), has been studied in order to ascertain details of the geometry of the oxime unit and to investigate any possible intermolecular interactions. The compound crystallizes in the non-centrosymmetric space group $Pca2_1$, with $Z' = 2$, in a unit cell of rather unusual shape. In the two independent molecules, which both have the *E* configuration at the C=N bond (Fig. 1), the key molecular dimensions are very similar (Table 1), although the inter-ring dihedral angles are slightly different, *viz*. 49.8 (2)° in molecule 1 (containing atom O17) and 52.1 (2)° in molecule 2 (containing O37).



(I)

Within the asymmetric unit, the molecules are linked by a nearly linear O—H···N hydrogen bond (Table 2). Similarly, atom O17 in the type 1 molecule at (*x*, *y*, *z*) acts as a hydrogen-bond donor to atom N37 in the type 2 molecule at (*x*, *y* − 1, *z*). Propagation by translation of these two hydrogen bonds then

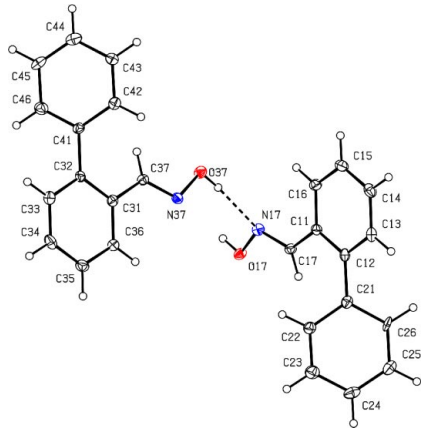


Figure 1
The two independent molecules of (I), showing the atom-labelling scheme and the N—H···O hydrogen bond within the asymmetric unit. Displacement parameters are drawn at the 30% probability level.

generates a $C_2^2(6)$ chain (Bernstein *et al.*, 1995), running parallel to the [010] direction (Fig. 2). Four chains of this type run through each unit cell; a pair of antiparallel chains lies in each of the two domains $0.03 < z < 0.49$ and $0.53 < z < 0.99$, but there are no direction-specific interactions between adjacent chains.

Experimental

Compound (I) was prepared by reaction of 2-phenylbenzaldehyde (Zaheer & French, 1944) with hydroxylamine in pyridine–ethanol solution, according to a published procedure (Forrester *et al.*, 1979). Crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation of a solution in ethanol (m.p. 390–391 K).

Crystal data

$C_{13}H_{11}NO$
$M_r = 197.23$
Orthorhombic, $Pca2_1$
$a = 14.3555$ (4) Å
$b = 4.4969$ (1) Å
$c = 31.4473$ (10) Å
$V = 2030.09$ (10) Å^3
$Z = 8$
$D_x = 1.291$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2356 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.08$ mm^{-1}
$T = 120$ (2) K
Needle, colourless
0.30 × 0.08 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
$T_{min} = 0.967$, $T_{max} = 0.994$
15 601 measured reflections
2356 independent reflections
1764 reflections with $I > 2\sigma(I)$
$R_{int} = 0.080$
$\theta_{max} = 27.5°$
$h = -18 \rightarrow 18$
$k = -5 \rightarrow 5$
$l = -40 \rightarrow 40$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.111$
$S = 1.03$
2356 reflections
273 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C11—C17	1.472 (5)	C31—C37	1.466 (5)
C17—N17	1.275 (4)	C37—N37	1.272 (4)
N17—O17	1.407 (4)	N37—O37	1.410 (4)
C11—C17—N17	121.8 (3)	C31—C37—N37	121.8 (3)
C17—N17—O17	110.8 (3)	C37—N37—O37	111.0 (3)
C12—C11—C17—N17	164.3 (3)	C32—C31—C37—N37	165.6 (3)
C11—C17—N17—O17	177.6 (3)	C31—C37—N37—O37	178.1 (3)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O17—H17A···N37^{i}	0.84	1.97	2.799 (3)	171
O37—H37A···N17	0.84	1.96	2.789 (4)	171

Symmetry code: (i) $x, y-1, z$.

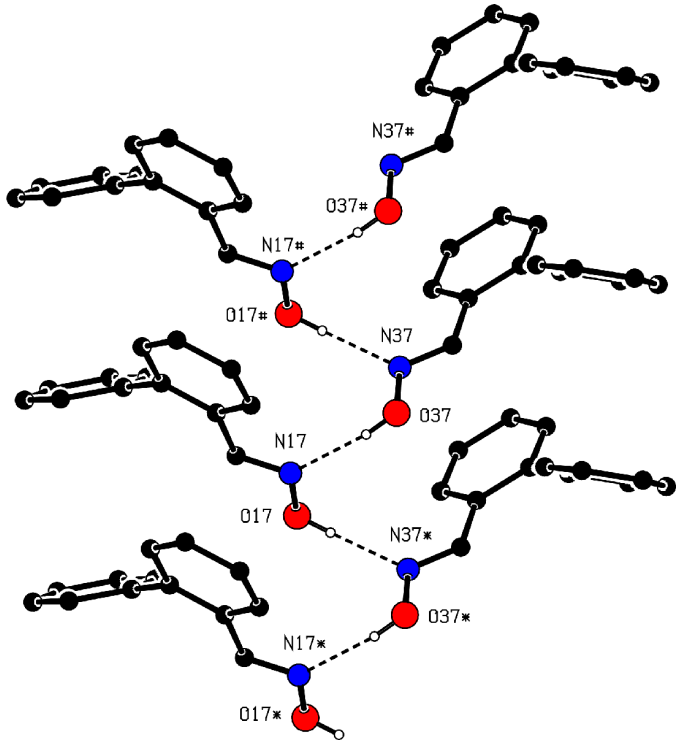


Figure 2
Part of the crystal structure of (I), showing the formation of a $C_2^2(6)$ chain running parallel to the [010] direction. For the sake of clarity, H atoms bonded to C atoms have been omitted; similarly, the unit-cell outline has been omitted because of its shape. Atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions $(x, y-1, z)$ and $(x, 1+y, z)$, respectively.

All H atoms were located in difference maps and then treated as riding atoms, with distances C—H = 0.95 Å and O—H = 0.84 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(O)$. In the absence of significant anomalous scattering, it was not possible to establish the correct orientation of the structure relative to the polar axis direction (Jones, 1986); hence the Friedel-equivalent reflections were merged prior to the final refinements.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL*97; molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97 and *PRPKAPPA* (Ferguson, 1999).

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